STRUCTURE AND INFRARED SPECTRA OF NEW AEROSOL PARTICLE FORMATION SEED CLUSTERS

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One of the largest unknowns in the understanding of aerosol particles is the structure and growth process that drives new particle formation, particularly from a *molecular* point of view. These particles typically form by the nucleation of water onto oxygenated byproducts of terpenes. Their structure and growth are dictated by the underlying interplay of hydrogen-bonding interactions of the organic molecules with water and water with itself. The presence of amine groups may further accelerate new particle formation. Here, we determine the structures of oxygenated byproducts of isoprene complexing with water and ammonia by employing infrared spectroscopy to reveal the important hydrogen-bonding interactions likely at play in larger clusters. We model the OH stretching region of the clusters' IR spectra through a suite of approaches that have favorable computational scaling and cost compared to standard anharmonic approaches. This acceleration allows us to consider the numerous candidate clusters and provide assignments. Finally, the wealth of spectral data (both theoretical and experimental) allows us to test the performance of data-driven spectroscopic models.